In the Abstract:

Please replace the following abstract for the pending abstract:

Provided is a <u>computer-implemented</u> method of ~~identifying~~ <u>analyzing a</u> <u>macromolecule for</u> potential binding sites ~~on a macromolecule comprising~~ <u>that includes</u>: ~~(a) for at least one organic fragment (ORF), conducting, at separate values of parameter *B*,~~ ~~two or more simulated annealing of chemical potential calculations using the ORF as the~~ ~~inserted solvent;~~ <u>positioning an instance of a computer representation of a molecule or</u> <u>molecular fragment at a plurality of sampling sites of the macromolecule; selecting a value</u> <u>of *B*, wherein $B = \mu'/kT + ln\langle N \rangle$, where μ' is the excess chemical potential, *k* is Boltzmann's</u> <u>constant, T is the absolute temperature, and $\langle N \rangle$ is the mean number of molecules of the</u> <u>molecule or molecular fragment; repositioning the instances of the molecule or molecular</u> <u>fragment; accepting or rejecting each instance of the repositioned molecule or molecular</u> <u>fragment based on the Metropolis sampling criteria using the computed binding energy</u> <u>compared to the selected value of *B*; repeating these steps at a lesser value of *B*;</u> ~~and (b)~~ ~~comparing converged solutions from step (a) to identify first locations at which the relevant~~ ~~ORF is strongly bound, thereby identifying candidate sites for binding ligand molecules~~ <u>outputting a list of unrejected instances of the molecule or molecular fragment, wherein the</u> <u>molecule or molecular fragment is an organic fragment; and outputting a list of one or more</u> <u>clusters of sampling sites, wherein the clusters of sampling sites include closely located or</u> <u>superimposed sampling sites associated with the unrejected instances of the molecule or</u> <u>molecular fragment.</u>